Fidelity and quantum phase transitions

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It is shown that the fidelity, a basic notion of quantum information science, may be used to characterize quantum phase transitions, regardless of what type of internal order is present in quantum many-body states. If the fidelity of two given states vanishes, then there are two cases: (1) they are in the same phase if the distinguishability results from irrelevant local information; or (2) they are in different phases if the distinguishability results from relevant long-distance information. The different effects of irrelevant and relevant information are quantified, which allows us to identify unstable and stable fixed points (in the sense of renormalization group theory). A physical implication of our results is the occurrence of the orthogonality catastrophe near the transition points.

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In recent decades, significant advances have been achieved in the study of quantum phase transitions (QPTs), both theoretically and experimentally, in systems such as high-T_c superconductors, fractional quantum Hall liquids, and quantum magnets [1]. Conventionally, QPTs are characterized by singularities of the ground state energy; first-order QPTs are characterized by discontinuities in the first derivative of the energy, whereas second-order (higher-order) QPTs are characterized by discontinuities in the second (higher) derivative of the energy. At singular points, the spectrum is gapless.

The focus of the traditional description of QPTs in condensed matter physics is a Hamiltonian and its spectrum. The most studied QPTs fit into the conventional Landau-Ginzburg-Wilson paradigm. A central concept is a local order parameter, whose non-zero value characterizes a symmetry-breaking phase, a unique feature which only exists for a system with infinite number of degrees of freedom, in contrast to QPTs resulting from a level crossing, which may happen in a finite size system. However, there exist phases that are not described by symmetry-breaking orders, which results in continuous QPTs beyond the Landau-Ginzburg-Wilson paradigm [2]. Indeed, such phase transitions exists between two phases with the *same* symmetry [3], between two states with *incompatible* symmetries [4], and even between two states with symmetry breaking, if the simultaneous changes of topological/quantum orders occur [5].

On the other hand, quantum information science brings about an emerging picture which studies QPTs from the ground state wave functions of systems. The cross fertilization of quantum many-body theory and quantum information science has led to fruitful outcomes. One aspect is the study of the possible role of entanglement in characterizing QPTs [6, 7, 8, 9]. Remarkably, for quantum spin chains, the von Neumann entropy, as a bipartite entanglement measure, exhibits qualitatively different behaviors at and off criticality [8]. Further, QPTs in spin chains characterized by local Hamiltonians with matrix product ground states exhibit a different type of QPTs from the standard paradigm, where the ground state energy remains analytic [10].

In this Letter, we investigate the role of the fidelity, a basic notion of quantum information science, in characterizing QPTs. As a distance measure, the fidelity describes how close two given quantum states are. Therefore, it is natural to expect that the fidelity may be used to characterize drastic changes in quantum states when systems undergo QPTs, regardless of what type of internal order is present in quantum many-body states. It is shown that the fidelity of two states vanishes due to different reasons depending on whether they are in the same phase or in different phases. For the former, the orthogonality results from irrelevant local information; for the latter, the orthogonality results from relevant long-distance information. One may identify unstable and stable fixed points by quantifying the effects of irrelevant and relevant information. We present examples exhibiting a second order phase transition, a critical line, a level crossing and an infinite order phase transition. An implication of our results is the orthogonality catastrophe near the transition points [11]. It is proper to stress here that Zanardi and Paunković [12] were the first to exploit the ground state overlap, which is equivalent to the fidelity at zero temperature, to detect QPTs in the Dicke model and the XY spin chain.

We consider a quantum system S described by a Hamiltonian $H(\lambda)$, with λ a control parameter [13]. The latter may be tuned to drive the system to undergo a QPT at some transition point λ_c. It should be stressed that the transition point may be of any type, caused by a level crossing, spontaneous symmetry breaking, or the occurrence of some exotic orders such as quantum/topological orders. Here we stress that the size of the system may be either thermodynamically large or finite, depending on the type of QPT. We first consider a system at zero temperature. Then the system is in a ground state. The main conclusion is as follows:

Proposition 1. If a quantum system S described by the Hamiltonian $H(\lambda)$ undergoes a QPT at a transition point λ_c, with $|\psi\rangle$ and $|\phi\rangle$ denoting, respectively, representative ground states in the phases $\lambda > \lambda_c$ and $\lambda < \lambda_c$, then we have $\langle\psi|\phi\rangle = 0$. That is, the fidelity $F(\psi, \phi) \equiv |\langle\psi|\phi\rangle|$ of two representative states from different phases vanishes. Conversely, if the fidelity of two given states $|\psi\rangle$ and $|\phi\rangle$ vanishes, i.e., they are orthogonal to each other, then either (1) they are in two different phases if the orthogonality results from relevant long-distance information present in the states; or (2) $|\psi\rangle$ and $|\phi\rangle$ belong to the same phase if the orthogonality results from irrelevant local (short-distance) information.

Proof. A representative state $|\psi\rangle$ in a given phase is reliably distinguishable from a representative state $|\phi\rangle$ in the other phase, due to the occurrence of different orders in different phases [14]. Here the distinguishability is understood in the sense of quantum measurements [15]. On the other hand, two non-orthogonal states cannot be reliably distinguished [15], as follows from the basic Postulate of Quantum Mechanics on quantum measurements. This implies that $\langle\psi|\phi\rangle = 0$. Conversely, if $|\psi\rangle$ and $|\phi\rangle$ are orthogonal to each other, then they are reliably distinguishable. Therefore, there must be some physical observable which may be exploited to distinguish the states and one may take this observable as an order parameter [16]. Therefore whether or not the two states are in the same phase depends on whether the difference unveiled by such an order parameter is quantitative or qualitative. In the former case, the distinguishability results from the short-distance details of the system, i.e., irrelevant local information of the system. Since the long-distance behavior of a system does not depend on the short-distance details of the system [2], so the two states share the same long-distance information and must be in the same phase. In the latter case, the distinguishability results from relevant long-distance information of the system, so the two states must belong to different phases.

To complete our characterization of QPTs in terms of the fidelity, it is necessary to quantify the different effects of irrelevant and relevant information. To this end, we restrict ourselves to consider systems exhibiting QPTs with symmetry-breaking orders and study the scaling behaviors of the fidelity with the system size L. We have

Proposition 2. For a quantum system of a large size L, the fidelity $F(\lambda, \lambda')$ scales as $[d(\lambda, \lambda')]^L$ [17], with $0 \leq d \leq 1$ some constant characterizing how fast the fidelity changes when the thermodynamic limit is approached. If λ and λ' are in different phases, then $d(\lambda_<, \lambda_>) \geq d(\lambda, \lambda') \geq d(\lambda_1, \lambda_2)$, where λ_1 and λ_2 are fixed points to which quantum states in two different phases flow under renormalization group (RG) transformations, and $\lambda_<$ and $\lambda_>$ approach the transition value λ_c from both sides (in the thermodynamic limit). If λ and λ' are in the same phase, then $d(\lambda, \lambda') \to 1$ as $\lambda \to \lambda'$.

Proof. It is well-known that symmetry-breaking orders emerge only in the thermodynamic limit. Therefore, the fidelity for any two ground states of a finite size system does not vanish, but is exponentially small due to the locality of order parameters when the size L is very large. Suppose the system flows to two different stable fixed points λ_1 and λ_2 under RG transformations [18]. Then we have $d(\lambda, \lambda') \geq d(\lambda_1, \lambda_2)$ if λ and λ' are in different phases, and λ and λ' flow to λ_1 and λ_2, respectively. This follows from the fact that two states at stable fixed points λ_1 and λ_2 are the most distinguishable states, since there is no suppression in order parameters caused from quantum fluctuations. The irrelevant short-distance information present in the states $\psi(\lambda)$ and $\psi(\lambda')$ only makes them less distinguishable. Indeed, two states in different phases possess different relevant long distance information, so they become more distinguishable when the short-distance information is washed away. The maximum is reached when λ and λ' approach the transition point λ_c from both sides, since strong quantum fluctuations makes them relatively less distinguishable among states in different phases. Thus $d(\lambda, \lambda') \leq d(\lambda_<, \lambda_>)$. However, $d(\lambda_<, \lambda_>)$ must be less than 1, because the short-distance (irrelevant) information cannot undo what results from the long-distance (relevant) information. In contrast, $d(\lambda, \lambda')$ smoothly approaches 1 if λ approaches λ' in the same phase. In fact, states in the same phase enjoy exactly the same relevant long-distance information, so they are indistinguishable at long-distance scales. However, the short-distance information makes them distinguishable. More precisely, $d(\lambda, \lambda')$ decreases with λ along a renormalization group flow for a fixed λ', if λ and λ' are in different phases, and $d(\lambda, \lambda')$ increases with λ, until it reaches 1 when $\lambda = \lambda'$, then it decreases with λ along a renormalization group flow for a fixed λ', if λ and λ' are in the same phase. Since $d(\lambda, \lambda')$ is continuous, and it is symmetric under exchange $\lambda \leftrightarrow \lambda'$, one may recognize unstable and stable fixed points as pinch points [19] and global minima, respectively.

Remark 1. One may extend the above argument to other types of QPTs. However, the exponential scaling of the fidelity with the size L is not necessarily valid. Actually, for QPTs resulting from level crossings, d only takes values 0 or 1. For QPTs in matrix product systems [10], the fidelity may exhibit a fast oscillating scaling behavior with an exponentially decaying envelope. Therefore *different scaling behaviors signal different types of QPTs.*

Now we turn to the finite temperature case. Then the system is in a mixed state, characterized by a density matrix ρ. A mixed state may be purified [15] if one introduces a reference system R, which has the same state space, e.g., another copy of S. That is, define a pure state $|SR\rangle$ for the joint system SR such that $\rho = \mathrm{tr}_R(|SR\rangle\langle SR|)$. Assume that orders present in ground states survive thermal fluctuations. Then we have

Proposition 3. If ρ and σ denote, respectively, two representative states of different phases for a quantum sys-

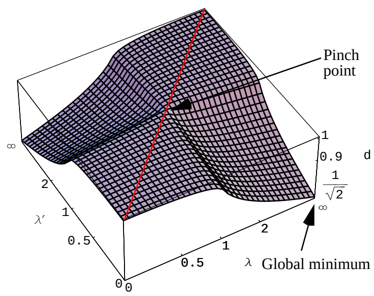

FIG. 1: (Color online) The scaling parameter d, which appears in the fidelity scaling $F(\lambda, \lambda') \sim d^L$, for the two states of quantum transverse Ising model as a function of λ and λ'. The transition point $\lambda_c = 1$ is characterized as a pinch point $(1, 1)$ and the two stable fixed points, to which all states in two phases flow, are characterized as the global minima at $(0, \infty)$ and $(\infty, 0)$. The red line denotes $d(\lambda, \lambda) = 1$.

tem S at finite temperature, then the fidelity $F(\rho, \sigma) = \mathrm{tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$ vanishes. Conversely, if the fidelity of two states ρ and σ is zero, i.e., $F(\rho, \sigma) = 0$, then either (1) ρ and σ are in two different phases and the orthogonality results from the qualitative difference of the relevant long-distance information; or (2) ρ and σ belong to the same phase and the orthogonality results from the quantitative difference of the irrelevant local information.

Proof. There is an alternative characterization of the fidelity due to Uhlmann's theorem [20], which states that $F(\rho, \sigma) = \max_{|\psi\rangle, |\phi\rangle} |\langle\psi|\phi\rangle|$, where the maximization is over all purifications $|\psi\rangle$ of ρ and $|\phi\rangle$ of σ in a joint system SR, with R being a copy of S. Since *any* purifications of ρ and σ must be orthogonal to each other, due to the fact that different orders in different phases make them reliably distinguishable. Combined with Uhlmann's theorem, one concludes that $F(\rho, \sigma) = 0$. Conversely, if $F(\rho, \sigma) = 0$, Uhlmann's theorem implies that the purifications of ρ and σ must be orthogonal to each other. Thus they must be reliably distinguishable. Since the reference system R is fictitious, and only the system S itself is accessible, so there must be some physical observable in the system S to characterize the distinguishability of the purifications. Thus we are led to conclusions along the same line of reasoning as *Proposition 1*.

Remark 2. The angle A between states ρ and σ defined by $A(\rho, \sigma) \equiv \arccos F(\rho, \sigma)$ is a metric [15]. That is, it is non-negative, symmetric and is equal to zero if and only if $\rho = \sigma$, and it obeys the triangle inequality: $A(\rho, \tau) \leq A(\rho, \sigma) + A(\sigma, \tau)$ for any states ρ, σ and τ. For brevity, we consider a finite (but large) size system at zero temperature. The angle A between two states at λ and λ', if one partitions the interval $[\lambda, \lambda']$ into N small pieces, satisfies $A \leq NA_N$, with A_N being the largest angle for N different pieces. If the two states are in different phases, then there exists at least one piece, for which the angle for the states at the ends of the piece is greater than A/N. Indeed, the angle for the piece across the transition point is $\sim \pi/2$. Instead, if the two states are in the same phase, then the interval may be partitioned into N pieces such that the angle between the ends of each piece is A/N, which can be as small as required.

One of physical implications of the above results is the Anderson orthogonality catastrophe around the transition point λ_c [11]. Indeed, no matter how close $\lambda_<$ and $\lambda_>$ are to the transition value λ_c, the corresponding ground states $|\psi(\lambda_<)\rangle$ and $|\psi(\lambda_>)\rangle$ must be *orthogonal* to each other, i.e., $\langle\psi(\lambda_<)|\psi(\lambda_>)\rangle = 0$ (in the thermodynamic limit). This was first discovered by Zanardi and Paunković [12] for the Dicke model and the XY spin chain, who also pointed out that the orthogonality catastrophe may reveal itself in the Loschmidt echo [21].

Quantum XY spin chain. The quantum XY spin chain is described by the Hamiltonian

$$H = -\sum_{j=-M}^{M} \left(\frac{1+\gamma}{2}\sigma_j^x\sigma_{j+1}^x + \frac{1-\gamma}{2}\sigma_j^y\sigma_{j+1}^y + \lambda\sigma_j^z\right). \quad (1)$$

Here σ_j^x, σ_j^y, and σ_j^z are the Pauli matrices at the j-th lattice site. The parameter γ denotes an anisotropy in the nearest-neighbor spin-spin interaction, whereas λ is an external magnetic field. The Hamiltonian (1) may be diagonalized as $H = \sum_k \Lambda_k(c_k^\dagger c_k - 1)$, where $\Lambda_k = \sqrt{(\lambda - \cos(2\pi k/L))^2 + \gamma^2 \sin^2(2\pi k/L)}$, with c_k and $c_k^\dagger$ denoting free fermionic modes and $L = 2M + 1$. The ground state $|\psi\rangle$ is the vacuum of all fermionic modes defined by $c_k|\psi\rangle = 0$, and may be written as $|\psi\rangle = \prod_{k=1}^{M}(\cos(\theta_k/2) - i\sin(\theta_k/2)c_k^\dagger c_{-k}^\dagger)|0\rangle_k|0\rangle_{-k}$, where $|0\rangle_k$ is the vacuum of the k-th mode, and θ_k is defined by $\cos\theta_k = (\cos(2\pi k/L) - \lambda)/\Lambda_k$. Therefore, the fidelity F for two states $|\psi(\lambda, \gamma)\rangle$ and $|\psi(\lambda', \gamma')\rangle$ takes the form,

$$F = \prod_{k=1}^{M} \cos\frac{\theta_k - \theta_k'}{2}, \quad (2)$$

where the prime denotes that the corresponding variables take their values at λ' and γ'. Obviously, $F = 1$ if $\lambda = \lambda'$ and $\gamma = \gamma'$. Generically, $\cos\frac{\theta_k - \theta_k'}{2} < 1$, therefore the fidelity decays very fast when λ and/or γ separate, respectively, from λ' and/or γ'.

Let us first consider the Heisenberg XX model in an external magnetic field ($\gamma = 0$), with a critical line characterized by $\lambda \in [0, 1)$. In this case, $\cos\theta_k = 1$ if $\cos(2\pi k/L) \geqslant \lambda$ and $\cos\theta_k = -1$ if $\cos(2\pi k/L) < \lambda$. Therefore, if both λ and λ' is greater than 1, then we have $F = 1$, consistent with the fact that the transition point $\lambda = 1$ for the Heisenberg XX model results from a level crossing. If $\lambda > 1$ and $\lambda' \leqslant 1$ or vice versa, then $F = 0$, consistent with *Proposition 1.* Suppose $\lambda < 1$ and $\lambda' < 1$, $F = 1$ only if λ and λ' are so close that there is no k satisfying $\lambda < \cos(2\pi k/L) < \lambda'$ or $\lambda' < \cos(2\pi k/L) < \lambda$.

In the thermodynamic limit, such a k always exists irrespective of λ and λ'. That is, $F = 0$ except for $\lambda = \lambda'$, indicating that there is a line of critical points $[0, 1)$, identified as the Luttinger liquids with dynamical critical exponent $z = 1$. We stress that the transition point $\lambda_c = 1$ with $z = 2$ controls the global features of the system.

Next consider the quantum transverse Ising universality class with the critical line $\gamma \neq 0$ and $\lambda = 1$. There is only one (second-order) critical point $\lambda_c = 1$ separating two gapful phases: (spin reversal) Z_2 symmetry-breaking and symmetric phases. In the thermodynamic limit, the scaling parameter d takes the form: $\ln d(\lambda, \lambda') = 1/(2\pi) \int_0^\pi d\alpha \ln \mathcal{F}(\lambda, \lambda'; \alpha)$, where $\mathcal{F}(\lambda, \lambda'; \alpha) = \cos[\vartheta(\lambda; \alpha) - \vartheta(\lambda'; \alpha)]/2$, with $\cos \vartheta(\lambda; \alpha) = (\cos\alpha - \lambda)/\sqrt{(\cos\alpha - \lambda)^2 + \gamma^2 \sin^2 \alpha}$. We plot d in Figure 1 for the transverse Ising model ($\gamma = 1$). One observes that the transition point $\lambda_c = 1$ is characterized as a pinch point $(1, 1)$ and that the two stable fixed points at $\lambda = 0$ and $\lambda = \infty$ are characterized as the global minima, which take value $1/\sqrt{2}$ at $(0, \infty)$ and $(\infty, 0)$.

The last case is the disorder-line, i.e., a unit circle given by $\lambda^2 + \gamma^2 = 1$ in the $\lambda - \gamma$ plane. We plot the scaling parameter d in Figure 2, from which one may read off that there are two transition points $(\pm 1, 0)$ and that there are two phases corresponding to the upper and lower semicircles, with $(0, \pm 1)$ as stable fixed points. The latter corresponds to two states with all spins aligning in the x and y directions, respectively. The system is dual to a spin 1/2 model with three-body interactions

$$H = \sum_i 2(g^2 - 1)\sigma_i^z \sigma_{i+1}^z - (1+g)^2 \sigma_i^x + (g-1)^2 \sigma_i^z \sigma_{i+1}^x \sigma_{i+2}^z, \tag{3}$$

with $\lambda = (1 - g^2)/(1 + g^2), \gamma = 2g/(1 + g^2)$. As shown in Ref. [10], the model exhibits a peculiar QPT in the thermodynamic limit, with divergent correlation length, vanishing energy gap, but analytic ground state energy. We emphasize that the parameter space should be compactified by identifying $g = +\infty$ and $g = -\infty$, due to the fact that $H(+\infty) = H(-\infty)$. Since ground states are matrix product states [10], it is straightforward to get the fidelity F for two states $|\psi(g)\rangle$ and $|\psi(g')\rangle$,

$$F = \frac{|(1 + \sqrt{gg'})^L + (1 - \sqrt{gg'})^L|}{\sqrt{[(1+g)^L + (1-g)^L][(1+g')^L + (1-g')^L]}}. \tag{4}$$

The fidelity F decays exponentially for two states in the same phase, but it is oscillating very fast with exponentially decaying envelope for two states in different phases. From this one may extract the scaling parameter d as $d(g, g') = \sqrt{1 + |gg'|}/\sqrt{(1 + |g|)(1 + |g'|)}$ if g and g' are in different phases, and $d(g, g') = (1 + \sqrt{|gg'|})/\sqrt{(1 + |g|)(1 + |g'|)}$ if g and g' are in the same phase. There are two transition points, i.e., $g = 0$ and ∞. All states for positive g flow to the product state ($g = 1$) with all spins aligning in the x direction, and all states for negative g flow to the cluster state [22] ($g = -1$).

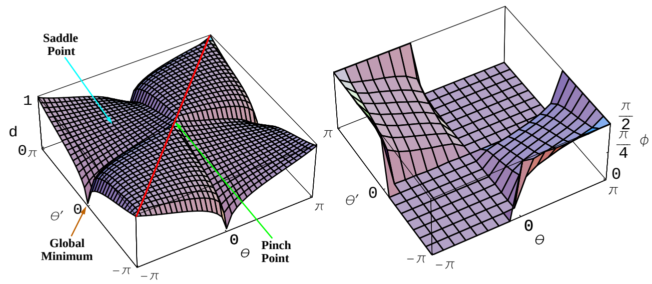

FIG. 2: (Color online) For the disorder line, $\lambda^2 + \gamma^2 = 1$ parameterized as $\lambda = \cos\theta$, and $\gamma = \sin\theta$, the fidelity $F(\theta, \theta')$ scales as $d^L cos(L\phi)$. Thus for $\phi \neq 0$, there is a sinusoidal oscillation with an exponential envelope in the fidelity. Left: The scaling parameter d as a function of θ and θ', displaying pinch points at $(\theta, \theta') = (0, 0)$ and (π, π), and saddle points at $(\pi/2, -\pi/2)$ and $(-\pi/2, \pi/2)$, if one identifies π with $-\pi$. The pinch points characterize the two transition points, while the saddle points characterize the stable fixed points, to which all states in two phases flow. The global minima at $(0, \pi)$ and $(\pi, 0)$ correspond to the transition points, due to the fact that both irrelevant and relevant information are different. Right: The phase ϕ as a function of θ and θ'.

In summary, we have established an intriguing connection between the fidelity and QPTs in particular and between quantum information science and condensed matter physics in general.

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